



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2023 – 06:34 PM EDT

PDB ID : 6DMF  
Title : Bacteroides ovatus mixed-linkage glucan utilization locus (MLGUL) SGBP-A with cellohexaose  
Authors : Koropatkin, N.M.; Bahr, C.M.  
Deposited on : 2018-06-05  
Resolution : 2.40 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

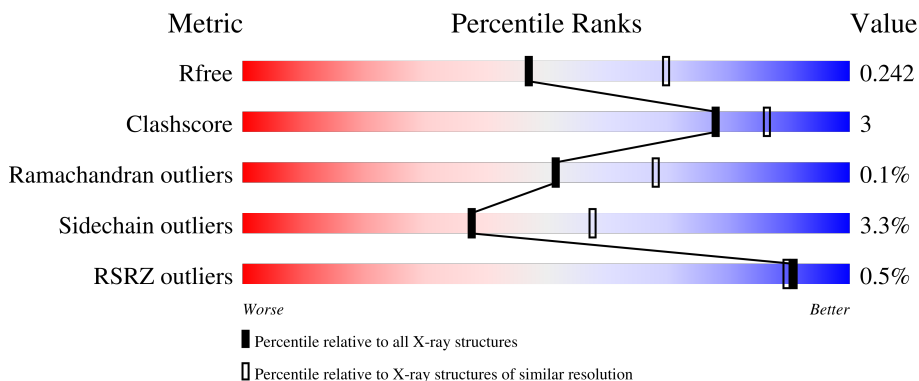
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	520	 91% 7% ..
1	B	520	 90% 9% ..
1	C	520	 91% 8% .
1	D	520	 90% 9% .
1	E	520	 91% 8% ..

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Mol	Chain	Length	Quality of chain
1	F	520	 92% 6% ..
1	G	520	 90% 8% ..
1	H	520	 89% 8% ..
1	I	520	 90% 7% ..
1	J	520	 89% 8% ..
2	K	5	 60% 40%
3	L	6	 17% 83%
3	M	6	 33% 67%
3	N	6	 67% 33%
3	O	6	 33% 67%
3	P	6	 50% 50%
3	Q	6	 50% 50%
3	R	6	 33% 67%
3	S	6	 50% 50%
3	T	6	 17% 83%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 42441 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called mixed-linkage glucan utilization locus (MLGUL) SGBP-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	513	4072	2572	676	804	20	0	0	0
1	B	516	4082	2579	680	803	20	0	0	0
1	C	512	4061	2563	675	803	20	0	0	0
1	D	519	4103	2592	683	808	20	0	0	0
1	E	517	4097	2588	681	808	20	0	0	0
1	F	514	4069	2571	677	801	20	0	0	0
1	G	512	4041	2552	673	796	20	0	0	0
1	H	514	4072	2574	677	801	20	0	0	0
1	I	510	4035	2551	672	792	20	0	0	0
1	J	512	4053	2561	674	798	20	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

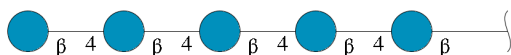
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ILE	-	expression tag	UNP A7LY27
B	39	ILE	-	expression tag	UNP A7LY27
C	39	ILE	-	expression tag	UNP A7LY27
D	39	ILE	-	expression tag	UNP A7LY27
E	39	ILE	-	expression tag	UNP A7LY27
F	39	ILE	-	expression tag	UNP A7LY27
G	39	ILE	-	expression tag	UNP A7LY27
H	39	ILE	-	expression tag	UNP A7LY27
I	39	ILE	-	expression tag	UNP A7LY27

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Chain	Residue	Modelled	Actual	Comment	Reference
J	39	ILE	-	expression tag	UNP A7LY27

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	K	5	56	30	26	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.

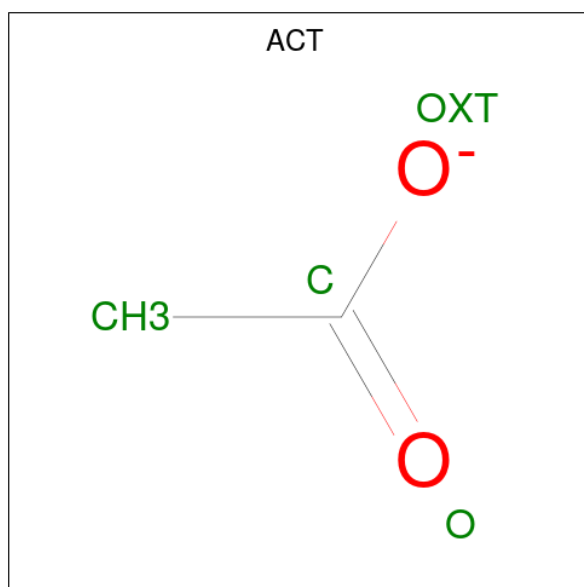


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	L	6	67	36	31	0	0	0
3	M	6	67	36	31	0	0	0
3	N	6	67	36	31	0	0	0
3	O	6	67	36	31	0	0	0
3	P	6	67	36	31	0	0	0
3	Q	6	67	36	31	0	0	0
3	R	6	67	36	31	0	0	0
3	S	6	67	36	31	0	0	0
3	T	6	67	36	31	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	I	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



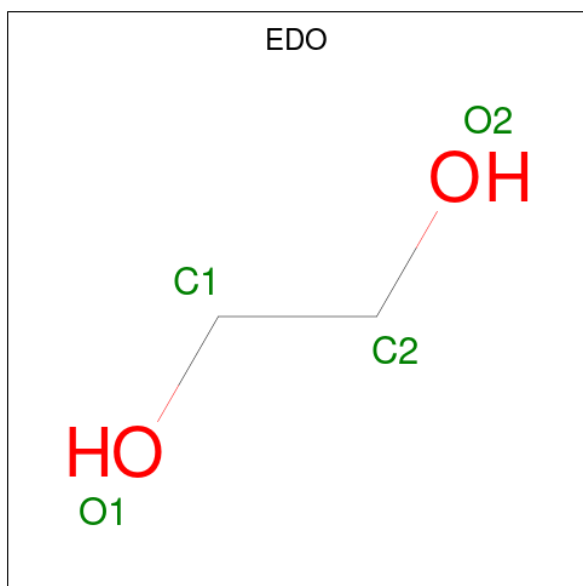
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	J	1	7	4	3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	4	2	2	0	0
7	B	1	4	2	2	0	0
7	B	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	D	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0
7	I	1	Total C O 4 2 2	0	0

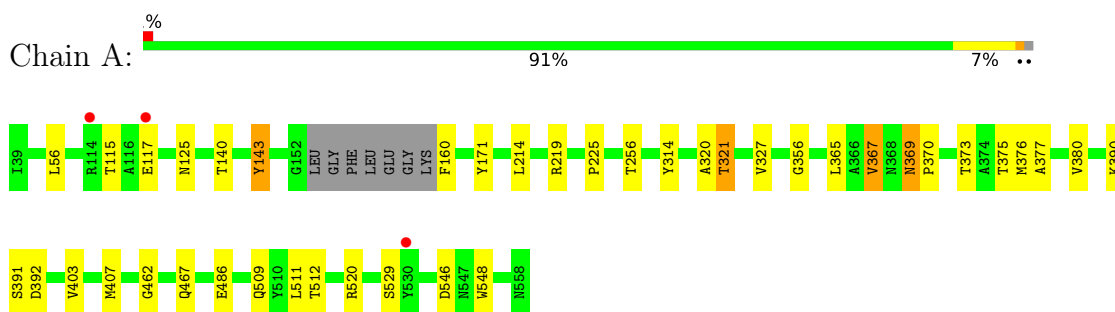
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	110	Total O 110 110	0	0
8	B	129	Total O 129 129	0	0
8	C	98	Total O 98 98	0	0
8	D	88	Total O 88 88	0	0
8	E	115	Total O 115 115	0	0
8	F	59	Total O 59 59	0	0
8	G	90	Total O 90 90	0	0
8	H	87	Total O 87 87	0	0
8	I	64	Total O 64 64	0	0
8	J	104	Total O 104 104	0	0

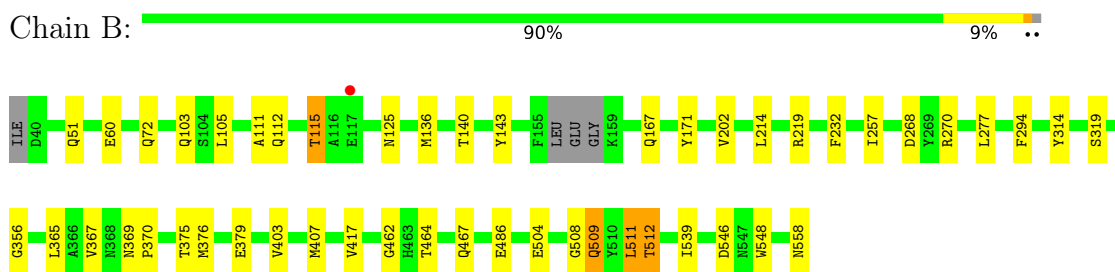
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

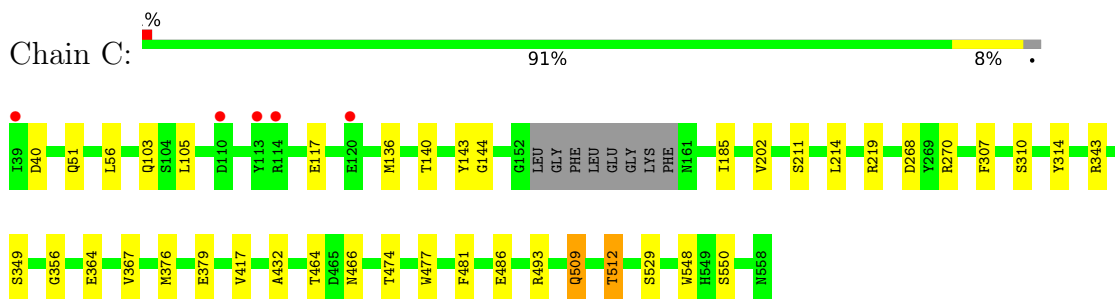
- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B



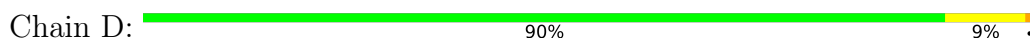
- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

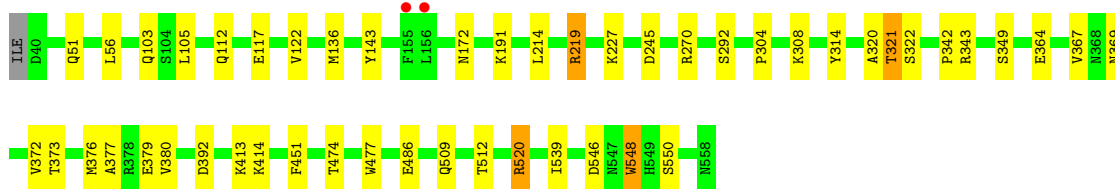


- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B



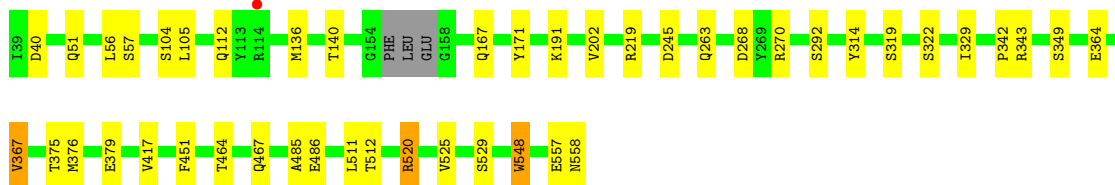
- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B





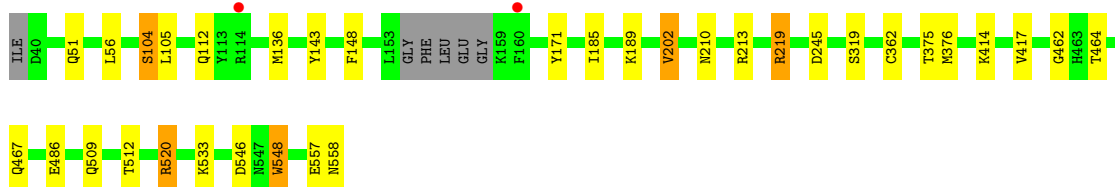
- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain E: 91% 8% ..



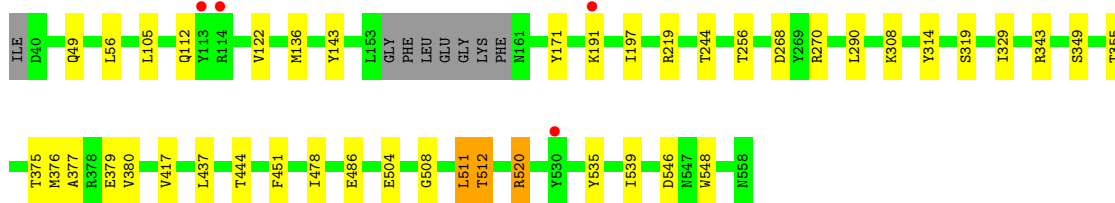
- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain F: 92% 6% ..



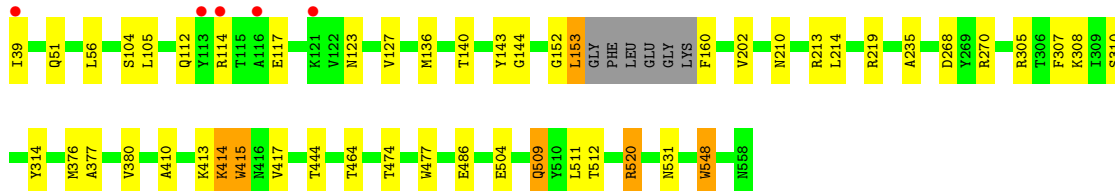
- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain G: 90% 8% ..



- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain H: 89% 8% ..



- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain O:  33% 67%



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain Q:  50% 50%



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain R:  33% 67%



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain S:  50% 50%



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain T:  17% 83%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.84Å 228.84Å 246.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.60 – 2.40 49.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.60-2.40) 89.6 (49.55-2.40)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.190 , 0.242 0.191 , 0.242	Depositor DCC
$R_{free}$ test set	14142 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	42441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3232e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ACT, BGC, EDO, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/4171	0.53	0/5671
1	B	0.36	0/4181	0.54	0/5684
1	C	0.35	0/4159	0.53	0/5655
1	D	0.35	0/4203	0.51	0/5715
1	E	0.37	0/4196	0.52	0/5703
1	F	0.33	0/4168	0.51	0/5668
1	G	0.34	0/4139	0.52	0/5631
1	H	0.37	0/4171	0.52	0/5672
1	I	0.34	0/4133	0.52	0/5619
1	J	0.36	0/4152	0.52	0/5646
All	All	0.35	0/41673	0.52	0/56664

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	F	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	219	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	270	ARG	Sidechain
1	F	219	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4072	0	3860	19	0
1	B	4082	0	3870	28	0
1	C	4061	0	3851	28	0
1	D	4103	0	3890	27	0
1	E	4097	0	3890	21	0
1	F	4069	0	3854	17	0
1	G	4041	0	3822	24	0
1	H	4072	0	3863	30	0
1	I	4035	0	3824	25	0
1	J	4053	0	3837	24	0
2	K	56	0	48	0	0
3	L	67	0	57	0	0
3	M	67	0	57	0	0
3	N	67	0	57	0	0
3	O	67	0	57	1	0
3	P	67	0	57	0	0
3	Q	67	0	57	0	0
3	R	67	0	57	0	0
3	S	67	0	57	0	0
3	T	67	0	57	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
5	E	4	0	3	0	0
5	F	4	0	3	0	0
5	H	4	0	3	0	0
5	I	4	0	3	0	0
5	J	4	0	3	0	0
6	A	14	0	20	0	0
6	B	14	0	20	0	0
6	J	7	0	10	0	0
7	A	4	0	6	0	0
7	B	8	0	12	0	0
7	C	12	0	18	1	0
7	D	4	0	6	0	0
7	E	16	0	24	1	0
7	G	20	0	30	2	0
7	H	4	0	6	0	0
7	I	4	0	6	0	0
8	A	110	0	0	1	0
8	B	129	0	0	2	0
8	C	98	0	0	4	0
8	D	88	0	0	0	0
8	E	115	0	0	0	0
8	F	59	0	0	0	0
8	G	90	0	0	1	0
8	H	87	0	0	0	0
8	I	64	0	0	2	0
8	J	104	0	0	0	0
All	All	42441	0	39307	232	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 232 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:TYR:O	1:D:520:ARG:NH1	1.60	1.31
1:H:51:GLN:NE2	1:H:104:SER:OG	1.87	1.07
1:G:143:TYR:O	1:G:520:ARG:NH1	2.05	0.89
1:G:268:ASP:OD1	1:G:270:ARG:HD3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:520:ARG:NH1	8:I:701:HOH:O	2.00	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/520 (98%)	487 (96%)	21 (4%)	1 (0%)	47	62
1	B	512/520 (98%)	492 (96%)	20 (4%)	0	100	100
1	C	508/520 (98%)	489 (96%)	19 (4%)	0	100	100
1	D	517/520 (99%)	500 (97%)	16 (3%)	1 (0%)	47	62
1	E	513/520 (99%)	493 (96%)	20 (4%)	0	100	100
1	F	510/520 (98%)	489 (96%)	20 (4%)	1 (0%)	47	62
1	G	508/520 (98%)	489 (96%)	19 (4%)	0	100	100
1	H	510/520 (98%)	483 (95%)	27 (5%)	0	100	100
1	I	504/520 (97%)	489 (97%)	14 (3%)	1 (0%)	47	62
1	J	508/520 (98%)	493 (97%)	14 (3%)	1 (0%)	47	62
All	All	5099/5200 (98%)	4904 (96%)	190 (4%)	5 (0%)	51	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	321	THR
1	F	189	LYS
1	A	321	THR
1	I	321	THR
1	J	144	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	436/441 (99%)	419 (96%)	17 (4%)	32	50
1	B	435/441 (99%)	419 (96%)	16 (4%)	34	53
1	C	435/441 (99%)	427 (98%)	8 (2%)	59	76
1	D	437/441 (99%)	422 (97%)	15 (3%)	37	56
1	E	438/441 (99%)	420 (96%)	18 (4%)	30	48
1	F	434/441 (98%)	420 (97%)	14 (3%)	39	59
1	G	430/441 (98%)	416 (97%)	14 (3%)	38	57
1	H	435/441 (99%)	418 (96%)	17 (4%)	32	50
1	I	430/441 (98%)	418 (97%)	12 (3%)	43	63
1	J	432/441 (98%)	418 (97%)	14 (3%)	39	59
All	All	4342/4410 (98%)	4197 (97%)	145 (3%)	38	57

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	512	THR
1	J	548	TRP
1	I	56	LEU
1	I	557	GLU
1	D	369	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	331	GLN
1	I	368	ASN
1	F	531	ASN
1	J	125	ASN
1	H	51	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

59 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	BGC	K	1	2	12,12,12	0.45	0	17,17,17	0.64	0
2	BGC	K	2	2	11,11,12	0.29	0	15,15,17	0.88	0
2	BGC	K	3	2	11,11,12	0.56	0	15,15,17	1.10	1 (6%)
2	BGC	K	4	2	11,11,12	0.56	0	15,15,17	0.83	0
2	BGC	K	5	2	11,11,12	0.58	0	15,15,17	1.26	1 (6%)
3	BGC	L	1	3	12,12,12	0.54	0	17,17,17	1.06	1 (5%)
3	BGC	L	2	3	11,11,12	0.31	0	15,15,17	0.88	0
3	BGC	L	3	3	11,11,12	0.57	0	15,15,17	1.96	2 (13%)
3	BGC	L	4	3	11,11,12	0.45	0	15,15,17	1.02	2 (13%)
3	BGC	L	5	3	11,11,12	0.36	0	15,15,17	1.10	2 (13%)
3	BGC	L	6	3	11,11,12	0.66	0	15,15,17	1.24	2 (13%)
3	BGC	M	1	3	12,12,12	0.50	0	17,17,17	0.87	0
3	BGC	M	2	3	11,11,12	0.29	0	15,15,17	0.83	0
3	BGC	M	3	3	11,11,12	0.64	0	15,15,17	0.88	1 (6%)
3	BGC	M	4	3	11,11,12	0.38	0	15,15,17	0.89	2 (13%)
3	BGC	M	5	3	11,11,12	0.38	0	15,15,17	0.83	1 (6%)
3	BGC	M	6	3	11,11,12	0.44	0	15,15,17	1.11	1 (6%)
3	BGC	N	1	3	12,12,12	0.48	0	17,17,17	0.90	1 (5%)
3	BGC	N	2	3	11,11,12	0.33	0	15,15,17	1.14	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BGC	N	3	3	11,11,12	0.43	0	15,15,17	0.97	0
3	BGC	N	4	3	11,11,12	0.31	0	15,15,17	0.79	0
3	BGC	N	5	3	11,11,12	0.51	0	15,15,17	0.86	0
3	BGC	N	6	3	11,11,12	0.40	0	15,15,17	1.04	0
3	BGC	O	1	3	12,12,12	0.56	0	17,17,17	0.96	0
3	BGC	O	2	3	11,11,12	0.40	0	15,15,17	1.14	2 (13%)
3	BGC	O	3	3	11,11,12	0.36	0	15,15,17	0.77	1 (6%)
3	BGC	O	4	3	11,11,12	0.38	0	15,15,17	0.69	0
3	BGC	O	5	3	11,11,12	0.48	0	15,15,17	1.26	3 (20%)
3	BGC	O	6	3	11,11,12	0.33	0	15,15,17	0.65	0
3	BGC	P	1	3	12,12,12	0.53	0	17,17,17	0.89	0
3	BGC	P	2	3	11,11,12	0.40	0	15,15,17	0.61	0
3	BGC	P	3	3	11,11,12	0.30	0	15,15,17	0.90	1 (6%)
3	BGC	P	4	3	11,11,12	0.51	0	15,15,17	0.85	1 (6%)
3	BGC	P	5	3	11,11,12	0.39	0	15,15,17	1.17	1 (6%)
3	BGC	P	6	3	11,11,12	0.40	0	15,15,17	0.77	0
3	BGC	Q	1	3	12,12,12	0.47	0	17,17,17	0.59	0
3	BGC	Q	2	3	11,11,12	0.39	0	15,15,17	0.78	0
3	BGC	Q	3	3	11,11,12	0.25	0	15,15,17	1.09	1 (6%)
3	BGC	Q	4	3	11,11,12	0.31	0	15,15,17	0.89	0
3	BGC	Q	5	3	11,11,12	0.41	0	15,15,17	1.29	1 (6%)
3	BGC	Q	6	3	11,11,12	0.42	0	15,15,17	1.01	1 (6%)
3	BGC	R	1	3	12,12,12	0.55	0	17,17,17	1.03	0
3	BGC	R	2	3	11,11,12	0.69	0	15,15,17	0.74	0
3	BGC	R	3	3	11,11,12	0.49	0	15,15,17	0.79	1 (6%)
3	BGC	R	4	3	11,11,12	0.38	0	15,15,17	0.81	1 (6%)
3	BGC	R	5	3	11,11,12	0.39	0	15,15,17	1.39	1 (6%)
3	BGC	R	6	3	11,11,12	0.33	0	15,15,17	0.90	1 (6%)
3	BGC	S	1	3	12,12,12	0.46	0	17,17,17	0.85	1 (5%)
3	BGC	S	2	3	11,11,12	0.37	0	15,15,17	1.71	2 (13%)
3	BGC	S	3	3	11,11,12	0.40	0	15,15,17	0.51	0
3	BGC	S	4	3	11,11,12	0.25	0	15,15,17	0.90	0
3	BGC	S	5	3	11,11,12	0.49	0	15,15,17	0.83	0
3	BGC	S	6	3	11,11,12	0.35	0	15,15,17	1.11	2 (13%)
3	BGC	T	1	3	12,12,12	0.47	0	17,17,17	0.81	1 (5%)
3	BGC	T	2	3	11,11,12	0.26	0	15,15,17	1.28	2 (13%)
3	BGC	T	3	3	11,11,12	0.61	0	15,15,17	0.70	0
3	BGC	T	4	3	11,11,12	0.36	0	15,15,17	0.87	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BGC	T	5	3	11,11,12	0.29	0	15,15,17	1.27	3 (20%)
3	BGC	T	6	3	11,11,12	0.36	0	15,15,17	0.96	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	K	1	2	-	1/2/22/22	0/1/1/1
2	BGC	K	2	2	-	0/2/19/22	0/1/1/1
2	BGC	K	3	2	-	0/2/19/22	0/1/1/1
2	BGC	K	4	2	-	0/2/19/22	0/1/1/1
2	BGC	K	5	2	-	2/2/19/22	0/1/1/1
3	BGC	L	1	3	-	0/2/22/22	0/1/1/1
3	BGC	L	2	3	-	0/2/19/22	0/1/1/1
3	BGC	L	3	3	-	1/2/19/22	0/1/1/1
3	BGC	L	4	3	-	1/2/19/22	0/1/1/1
3	BGC	L	5	3	-	2/2/19/22	0/1/1/1
3	BGC	L	6	3	-	1/2/19/22	0/1/1/1
3	BGC	M	1	3	-	2/2/22/22	0/1/1/1
3	BGC	M	2	3	-	2/2/19/22	0/1/1/1
3	BGC	M	3	3	-	0/2/19/22	0/1/1/1
3	BGC	M	4	3	-	1/2/19/22	0/1/1/1
3	BGC	M	5	3	-	2/2/19/22	0/1/1/1
3	BGC	M	6	3	-	2/2/19/22	0/1/1/1
3	BGC	N	1	3	-	2/2/22/22	0/1/1/1
3	BGC	N	2	3	-	0/2/19/22	0/1/1/1
3	BGC	N	3	3	-	0/2/19/22	0/1/1/1
3	BGC	N	4	3	-	0/2/19/22	0/1/1/1
3	BGC	N	5	3	-	2/2/19/22	0/1/1/1
3	BGC	N	6	3	-	2/2/19/22	0/1/1/1
3	BGC	O	1	3	-	2/2/22/22	0/1/1/1
3	BGC	O	2	3	-	0/2/19/22	0/1/1/1
3	BGC	O	3	3	-	0/2/19/22	0/1/1/1
3	BGC	O	4	3	-	1/2/19/22	0/1/1/1
3	BGC	O	5	3	-	0/2/19/22	0/1/1/1
3	BGC	O	6	3	-	0/2/19/22	0/1/1/1
3	BGC	P	1	3	-	2/2/22/22	0/1/1/1
3	BGC	P	2	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	P	3	3	-	2/2/19/22	0/1/1/1
3	BGC	P	4	3	-	0/2/19/22	0/1/1/1
3	BGC	P	5	3	-	2/2/19/22	0/1/1/1
3	BGC	P	6	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	1	3	-	0/2/22/22	0/1/1/1
3	BGC	Q	2	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	3	3	-	2/2/19/22	0/1/1/1
3	BGC	Q	4	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	5	3	-	1/2/19/22	0/1/1/1
3	BGC	Q	6	3	-	1/2/19/22	0/1/1/1
3	BGC	R	1	3	-	0/2/22/22	0/1/1/1
3	BGC	R	2	3	-	0/2/19/22	0/1/1/1
3	BGC	R	3	3	-	2/2/19/22	0/1/1/1
3	BGC	R	4	3	-	0/2/19/22	0/1/1/1
3	BGC	R	5	3	-	2/2/19/22	0/1/1/1
3	BGC	R	6	3	-	2/2/19/22	0/1/1/1
3	BGC	S	1	3	-	2/2/22/22	0/1/1/1
3	BGC	S	2	3	-	2/2/19/22	0/1/1/1
3	BGC	S	3	3	-	0/2/19/22	0/1/1/1
3	BGC	S	4	3	-	0/2/19/22	0/1/1/1
3	BGC	S	5	3	-	1/2/19/22	0/1/1/1
3	BGC	S	6	3	-	2/2/19/22	0/1/1/1
3	BGC	T	1	3	-	1/2/22/22	0/1/1/1
3	BGC	T	2	3	-	0/2/19/22	0/1/1/1
3	BGC	T	3	3	-	0/2/19/22	0/1/1/1
3	BGC	T	4	3	-	0/2/19/22	0/1/1/1
3	BGC	T	5	3	-	2/2/19/22	0/1/1/1
3	BGC	T	6	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	3	BGC	C1-O5-C5	5.75	119.98	112.19
3	S	2	BGC	C1-O5-C5	5.28	119.35	112.19
3	R	5	BGC	C1-O5-C5	3.90	117.48	112.19
3	M	6	BGC	O5-C5-C6	3.40	112.53	107.20
3	T	2	BGC	C1-O5-C5	3.37	116.75	112.19

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

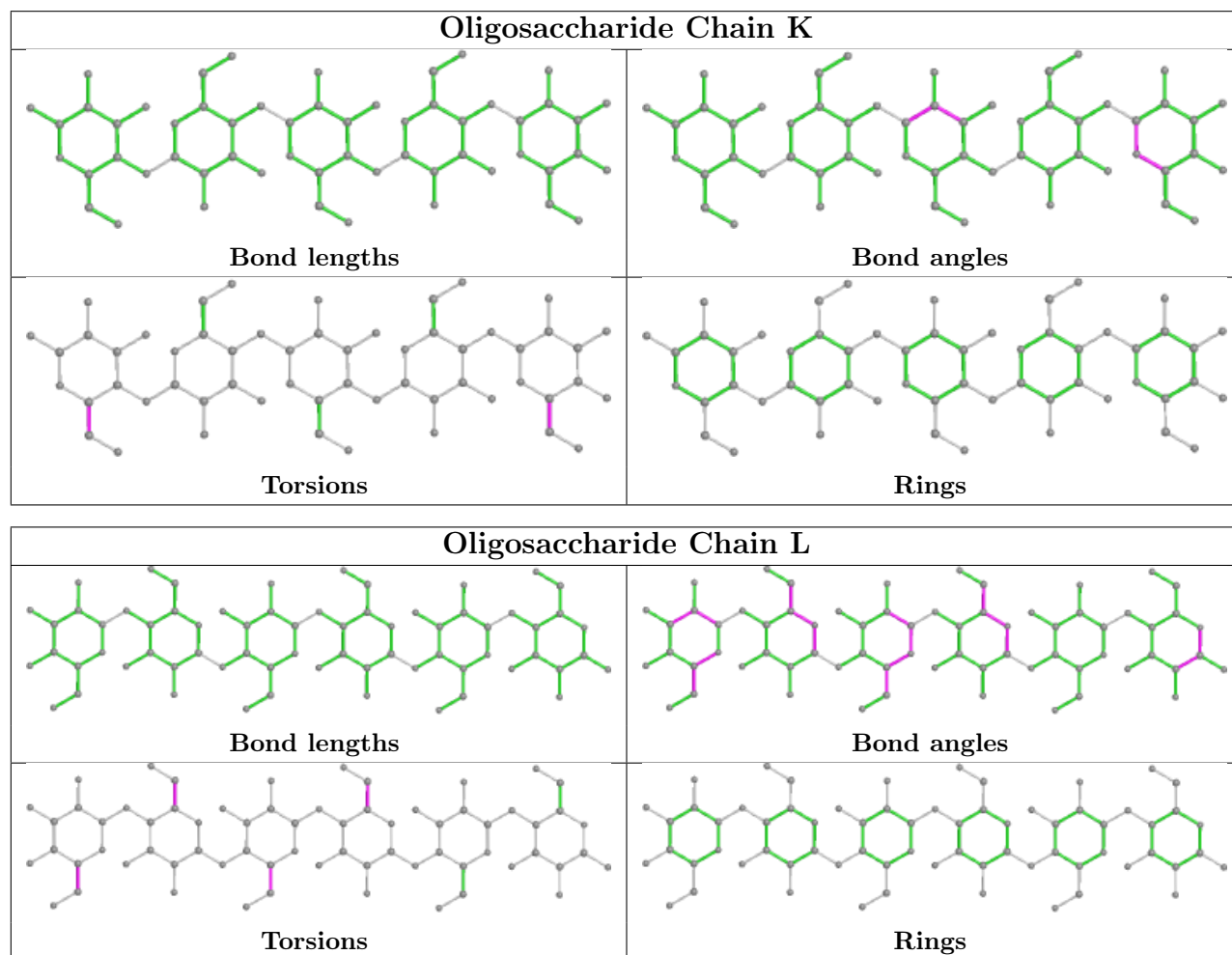
Mol	Chain	Res	Type	Atoms
3	R	6	BGC	O5-C5-C6-O6
3	M	5	BGC	O5-C5-C6-O6
2	K	5	BGC	O5-C5-C6-O6
3	P	3	BGC	O5-C5-C6-O6
3	S	6	BGC	O5-C5-C6-O6

There are no ring outliers.

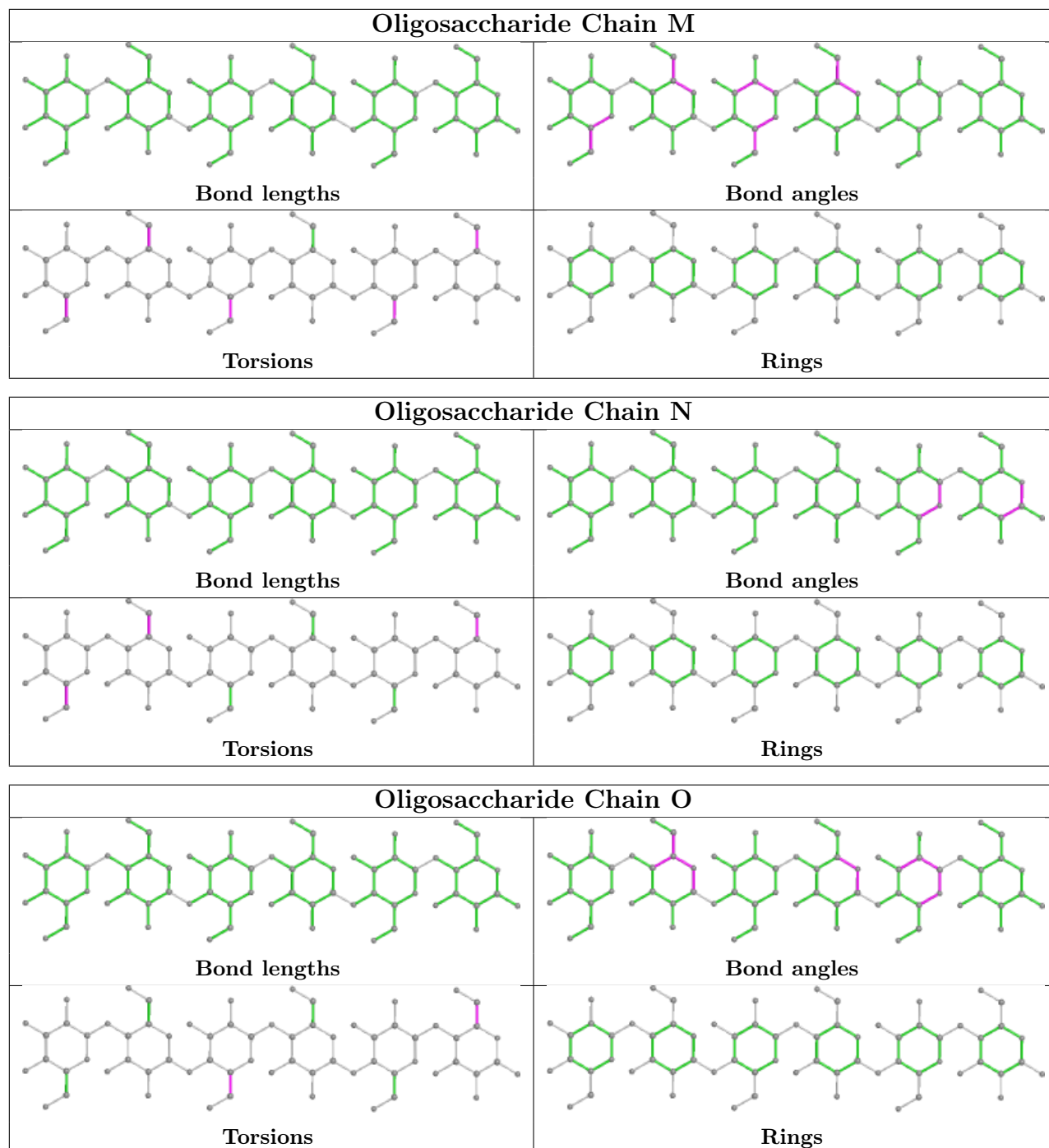
1 monomer is involved in 1 short contact:

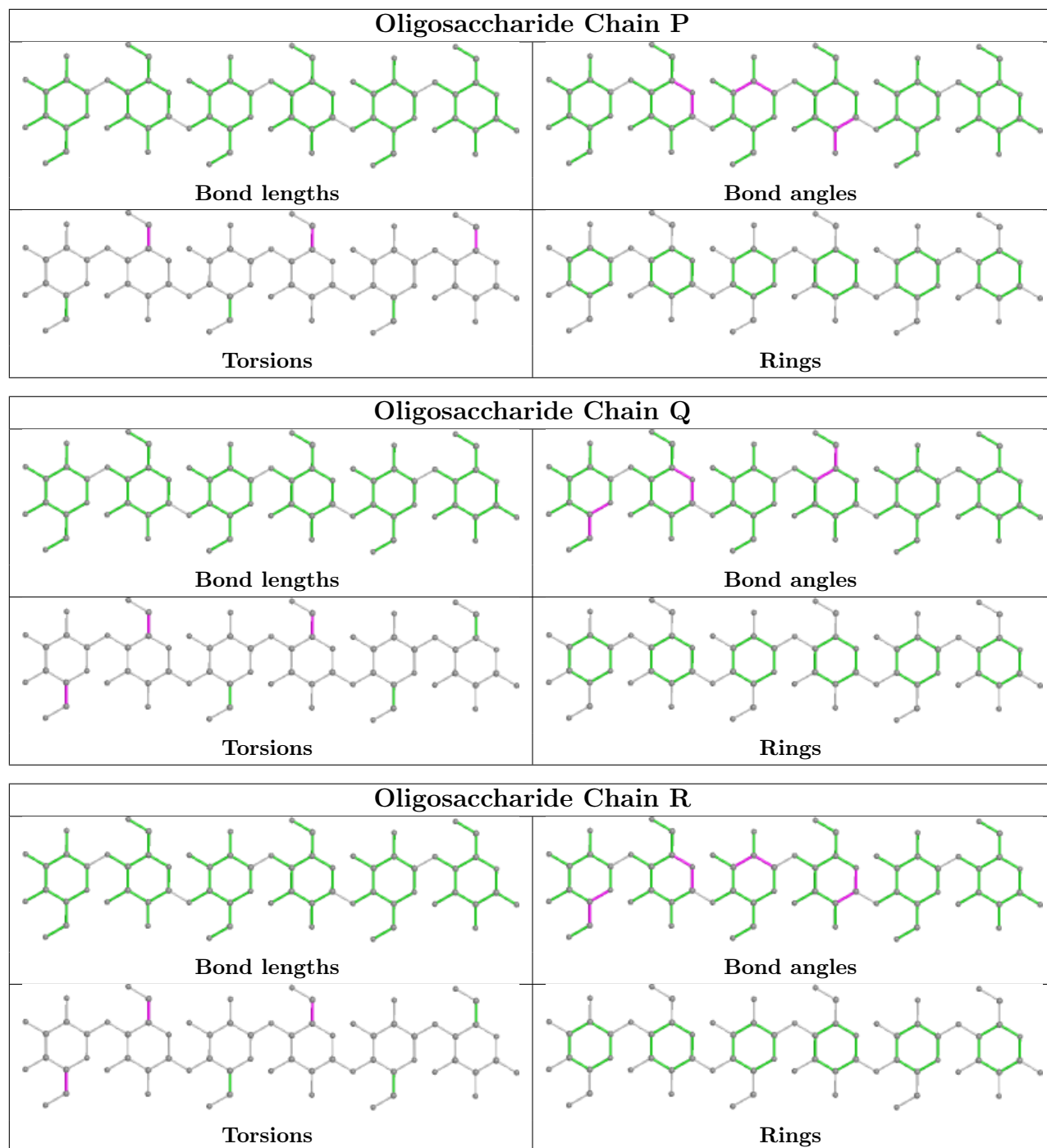
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	BGC	1	0

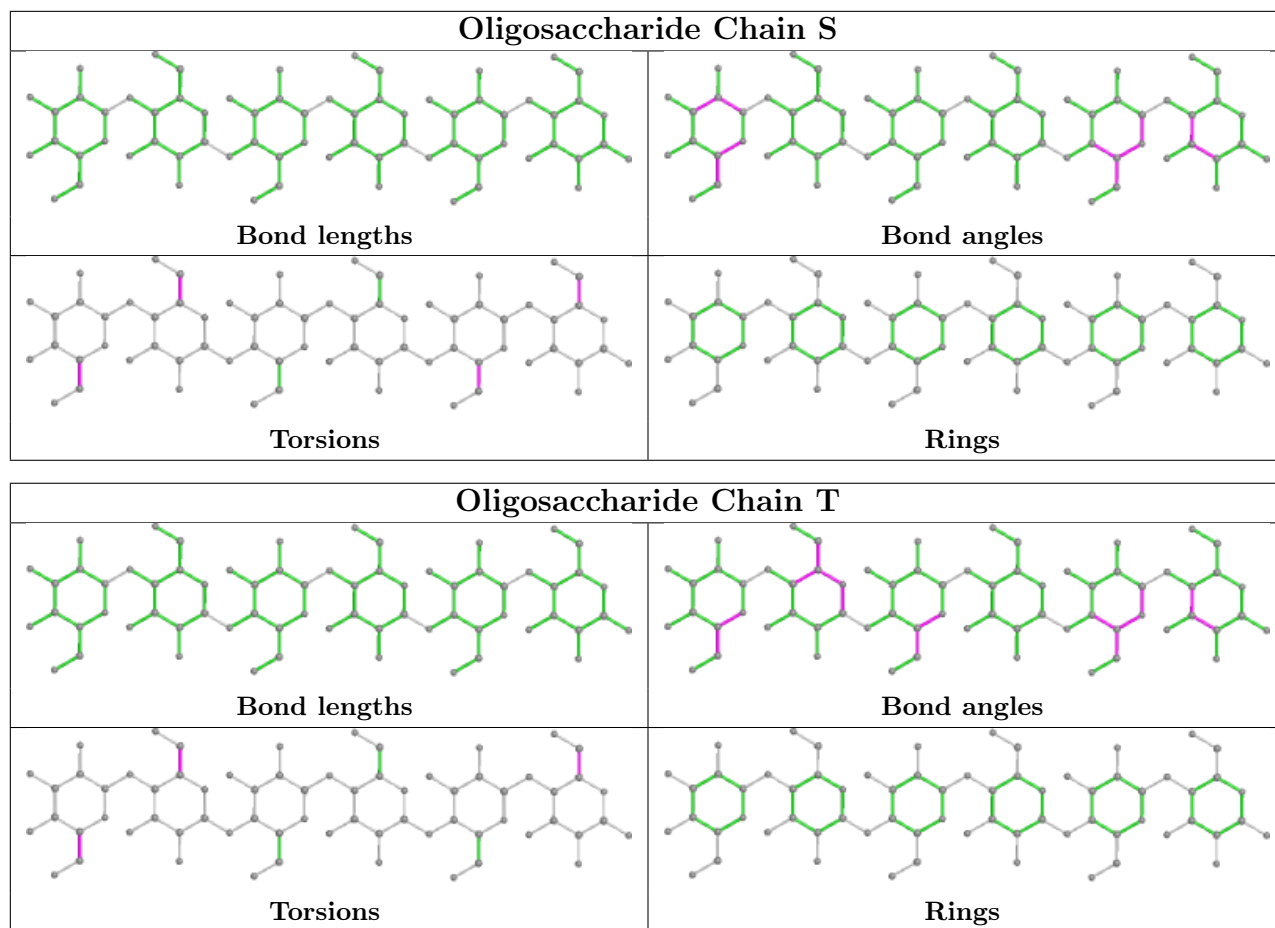
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 10 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	ACT	A	607	-	3,3,3	0.73	0	3,3,3	0.66	0
7	EDO	B	612	-	3,3,3	0.45	0	2,2,2	0.25	0
7	EDO	G	609	-	3,3,3	0.50	0	2,2,2	0.19	0
7	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.22	0
7	EDO	G	608	-	3,3,3	0.77	0	2,2,2	0.83	0
5	ACT	I	608	-	3,3,3	0.77	0	3,3,3	0.64	0
6	PEG	J	609	-	6,6,6	0.44	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	H	609	-	3,3,3	0.45	0	2,2,2	0.26	0
6	PEG	A	608	-	6,6,6	0.58	0	5,5,5	0.77	0
5	ACT	J	608	-	3,3,3	0.77	0	3,3,3	0.83	0
7	EDO	E	612	-	3,3,3	0.52	0	2,2,2	0.21	0
7	EDO	E	609	-	3,3,3	0.53	0	2,2,2	0.17	0
5	ACT	C	608	-	3,3,3	0.72	0	3,3,3	0.79	0
7	EDO	G	612	-	3,3,3	0.48	0	2,2,2	0.34	0
7	EDO	E	610	-	3,3,3	0.55	0	2,2,2	0.38	0
7	EDO	C	611	-	3,3,3	0.50	0	2,2,2	0.12	0
6	PEG	B	610	-	6,6,6	0.48	0	5,5,5	0.19	0
5	ACT	D	608	-	3,3,3	0.72	0	3,3,3	0.89	0
5	ACT	E	608	-	3,3,3	0.76	0	3,3,3	0.73	0
6	PEG	A	609	-	6,6,6	0.48	0	5,5,5	0.17	0
6	PEG	B	609	-	6,6,6	0.53	0	5,5,5	0.29	0
7	EDO	I	609	-	3,3,3	0.52	0	2,2,2	0.21	0
5	ACT	B	608	-	3,3,3	0.87	0	3,3,3	0.49	0
7	EDO	C	609	-	3,3,3	0.49	0	2,2,2	0.21	0
7	EDO	G	611	-	3,3,3	0.48	0	2,2,2	0.23	0
5	ACT	H	608	-	3,3,3	0.77	0	3,3,3	0.74	0
7	EDO	C	610	-	3,3,3	0.45	0	2,2,2	0.25	0
7	EDO	E	611	-	3,3,3	0.50	0	2,2,2	0.15	0
7	EDO	D	609	-	3,3,3	0.45	0	2,2,2	0.23	0
7	EDO	G	610	-	3,3,3	0.49	0	2,2,2	0.27	0
7	EDO	B	611	-	3,3,3	0.47	0	2,2,2	0.19	0
5	ACT	F	608	-	3,3,3	0.75	0	3,3,3	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	612	-	-	0/1/1/1	-
7	EDO	G	609	-	-	1/1/1/1	-
7	EDO	A	610	-	-	1/1/1/1	-
7	EDO	G	608	-	-	0/1/1/1	-
6	PEG	J	609	-	-	2/4/4/4	-
7	EDO	H	609	-	-	1/1/1/1	-
6	PEG	A	608	-	-	2/4/4/4	-
7	EDO	E	612	-	-	1/1/1/1	-
7	EDO	E	609	-	-	0/1/1/1	-
7	EDO	G	612	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	E	610	-	-	1/1/1/1	-
7	EDO	C	611	-	-	1/1/1/1	-
6	PEG	B	610	-	-	2/4/4/4	-
6	PEG	A	609	-	-	2/4/4/4	-
6	PEG	B	609	-	-	2/4/4/4	-
7	EDO	I	609	-	-	1/1/1/1	-
7	EDO	C	609	-	-	0/1/1/1	-
7	EDO	G	611	-	-	1/1/1/1	-
7	EDO	C	610	-	-	1/1/1/1	-
7	EDO	E	611	-	-	0/1/1/1	-
7	EDO	D	609	-	-	1/1/1/1	-
7	EDO	G	610	-	-	0/1/1/1	-
7	EDO	B	611	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	609	PEG	O1-C1-C2-O2
6	A	608	PEG	O2-C3-C4-O4
6	A	609	PEG	O2-C3-C4-O4
7	A	610	EDO	O1-C1-C2-O2
7	B	611	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	608	EDO	2	0
7	E	610	EDO	1	0
7	C	611	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	513/520 (98%)	-0.62	3 (0%) 89 88	19, 30, 53, 79	0
1	B	516/520 (99%)	-0.70	1 (0%) 95 94	16, 27, 46, 78	0
1	C	512/520 (98%)	-0.57	5 (0%) 82 80	19, 32, 58, 87	0
1	D	519/520 (99%)	-0.59	2 (0%) 92 91	18, 34, 55, 79	0
1	E	517/520 (99%)	-0.63	1 (0%) 95 94	19, 31, 52, 75	0
1	F	514/520 (98%)	-0.52	2 (0%) 92 91	20, 39, 63, 81	0
1	G	512/520 (98%)	-0.61	4 (0%) 86 84	21, 32, 56, 72	0
1	H	514/520 (98%)	-0.53	5 (0%) 82 80	20, 35, 56, 76	0
1	I	510/520 (98%)	-0.55	2 (0%) 92 91	24, 39, 59, 70	0
1	J	512/520 (98%)	-0.59	3 (0%) 89 88	19, 34, 58, 85	0
All	All	5139/5200 (98%)	-0.59	28 (0%) 91 89	16, 33, 58, 87	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	160	PHE	3.7
1	C	39	ILE	3.4
1	C	114	ARG	3.1
1	D	155	PHE	2.9
1	A	114	ARG	2.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	L	1	12/12	0.81	0.21	53,58,62,65	0
3	BGC	O	1	12/12	0.83	0.21	53,63,71,75	0
3	BGC	N	1	12/12	0.87	0.17	54,62,64,71	0
3	BGC	S	1	12/12	0.87	0.17	51,62,72,74	0
3	BGC	M	1	12/12	0.88	0.23	54,68,73,74	0
3	BGC	T	1	12/12	0.88	0.15	53,57,64,68	0
3	BGC	Q	1	12/12	0.89	0.13	56,59,64,65	0
3	BGC	R	2	11/12	0.89	0.13	49,53,57,57	0
3	BGC	R	1	12/12	0.90	0.16	57,63,66,66	0
2	BGC	K	1	12/12	0.90	0.16	50,59,66,66	0
3	BGC	M	2	11/12	0.91	0.14	44,47,58,64	0
3	BGC	N	2	11/12	0.91	0.14	53,55,58,60	0
3	BGC	P	6	11/12	0.92	0.18	63,68,75,76	0
3	BGC	P	1	12/12	0.92	0.14	61,67,71,76	0
3	BGC	P	2	11/12	0.93	0.11	49,57,60,61	0
3	BGC	P	3	11/12	0.93	0.15	60,62,68,74	0
3	BGC	L	6	11/12	0.93	0.13	42,47,51,53	0
3	BGC	M	3	11/12	0.93	0.11	40,43,45,47	0
3	BGC	P	5	11/12	0.94	0.12	56,60,66,70	0
3	BGC	N	6	11/12	0.94	0.11	53,58,63,65	0
3	BGC	M	6	11/12	0.94	0.11	44,48,52,62	0
3	BGC	Q	2	11/12	0.94	0.10	44,46,49,54	0
3	BGC	Q	6	11/12	0.94	0.12	41,44,49,51	0
3	BGC	L	2	11/12	0.94	0.11	40,43,50,57	0
3	BGC	L	3	11/12	0.94	0.11	33,35,42,43	0
3	BGC	N	3	11/12	0.94	0.09	46,50,52,54	0
3	BGC	S	2	11/12	0.94	0.10	42,45,51,60	0
3	BGC	P	4	11/12	0.94	0.11	52,56,59,59	0
3	BGC	T	2	11/12	0.94	0.12	41,48,52,62	0
3	BGC	T	5	11/12	0.94	0.11	36,39,46,48	0
3	BGC	N	5	11/12	0.95	0.10	50,54,63,65	0
3	BGC	L	5	11/12	0.95	0.12	34,38,42,46	0
3	BGC	R	3	11/12	0.95	0.13	46,47,57,59	0
3	BGC	R	6	11/12	0.95	0.12	50,54,60,60	0
2	BGC	K	5	11/12	0.95	0.10	38,42,48,50	0
3	BGC	O	2	11/12	0.95	0.14	43,51,57,58	0
3	BGC	S	5	11/12	0.95	0.13	39,43,46,49	0

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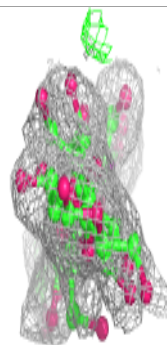
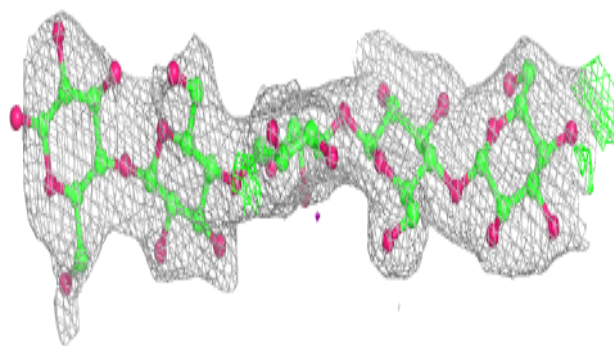
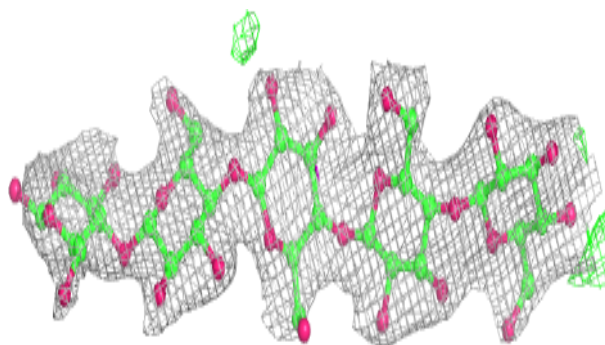
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BGC	O	3	11/12	0.95	0.10	40,41,48,48	0
2	BGC	K	3	11/12	0.95	0.11	37,45,53,58	0
3	BGC	T	4	11/12	0.95	0.10	32,34,36,36	0
3	BGC	N	4	11/12	0.95	0.10	46,52,57,58	0
3	BGC	T	6	11/12	0.95	0.18	45,49,57,64	0
2	BGC	K	2	11/12	0.96	0.09	47,49,53,55	0
3	BGC	S	3	11/12	0.96	0.08	39,42,47,50	0
3	BGC	S	4	11/12	0.96	0.10	36,38,42,45	0
3	BGC	M	4	11/12	0.96	0.10	33,39,41,42	0
3	BGC	Q	3	11/12	0.96	0.12	37,41,48,59	0
3	BGC	R	4	11/12	0.96	0.10	45,48,55,62	0
3	BGC	R	5	11/12	0.96	0.10	46,49,52,60	0
3	BGC	Q	5	11/12	0.96	0.10	37,39,44,47	0
3	BGC	O	6	11/12	0.96	0.11	38,40,43,45	0
3	BGC	L	4	11/12	0.97	0.11	32,33,35,35	0
3	BGC	S	6	11/12	0.97	0.12	41,44,47,52	0
3	BGC	M	5	11/12	0.97	0.09	39,42,43,45	0
2	BGC	K	4	11/12	0.97	0.07	35,36,38,40	0
3	BGC	T	3	11/12	0.97	0.08	36,39,42,49	0
3	BGC	O	4	11/12	0.97	0.10	33,36,40,42	0
3	BGC	O	5	11/12	0.97	0.09	36,40,47,51	0
3	BGC	Q	4	11/12	0.97	0.08	32,37,41,42	0

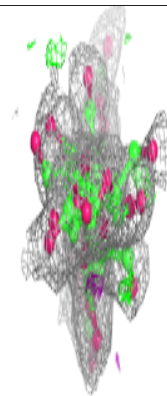
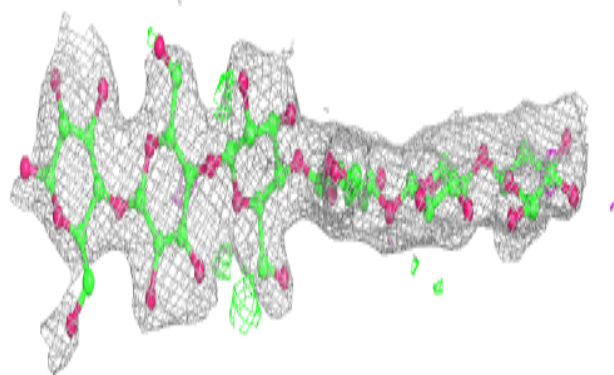
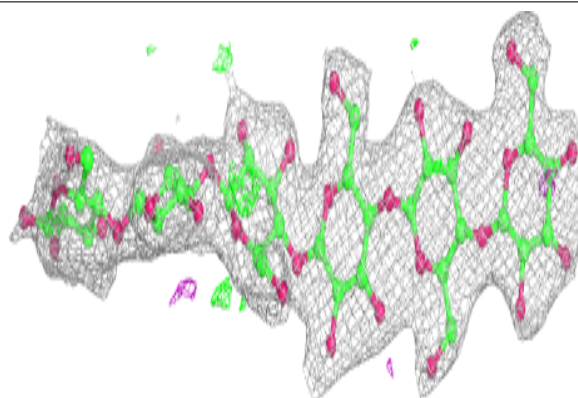
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain K:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

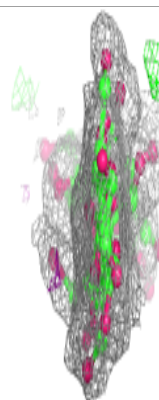
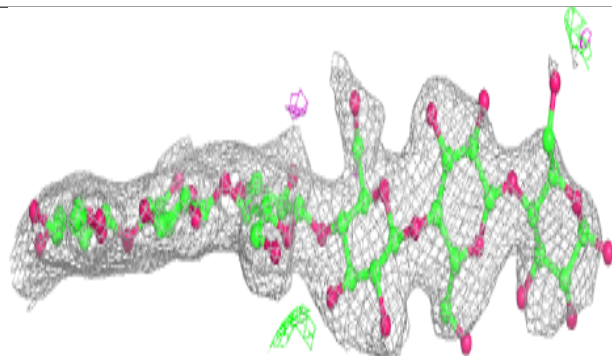
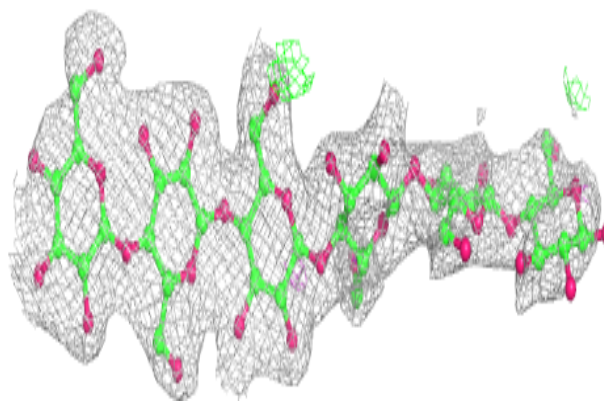
**Electron density around Chain L:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

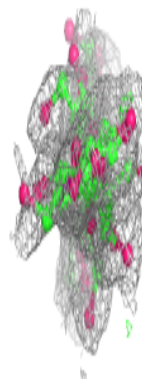
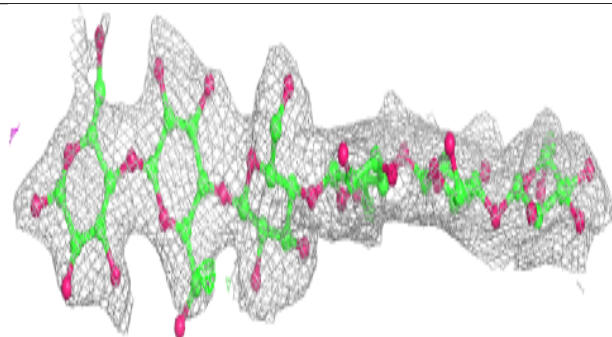
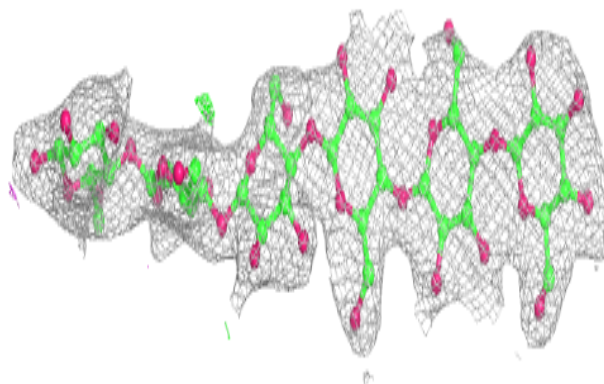


**Electron density around Chain M:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

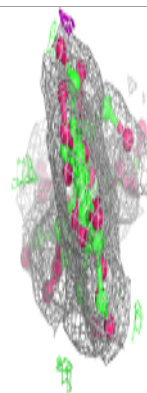
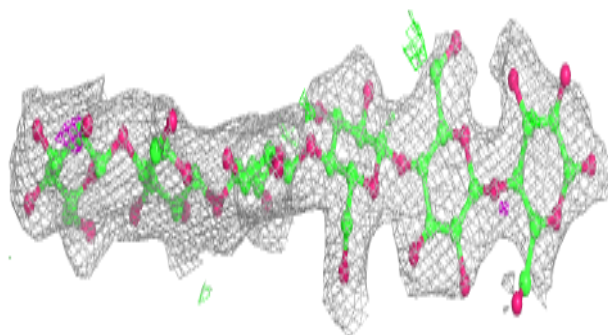
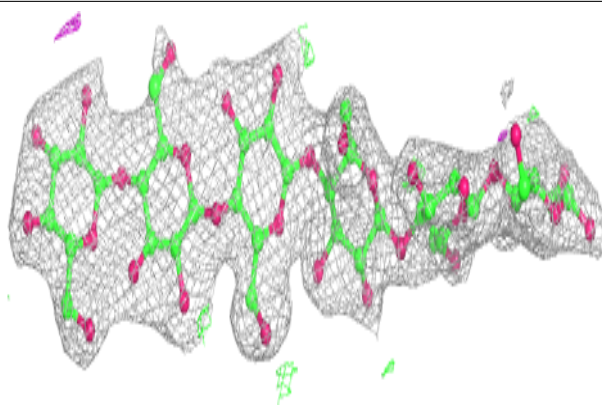
**Electron density around Chain N:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

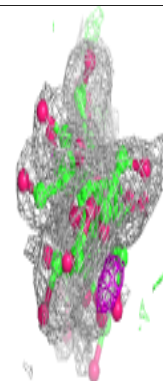
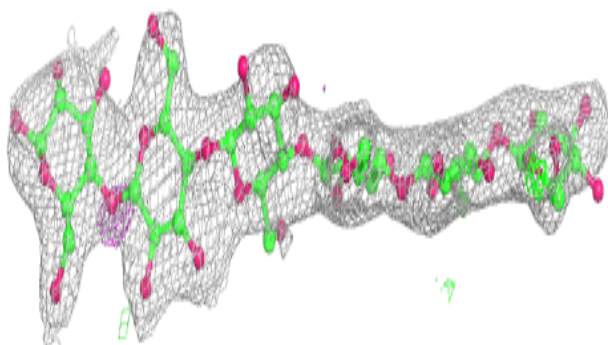
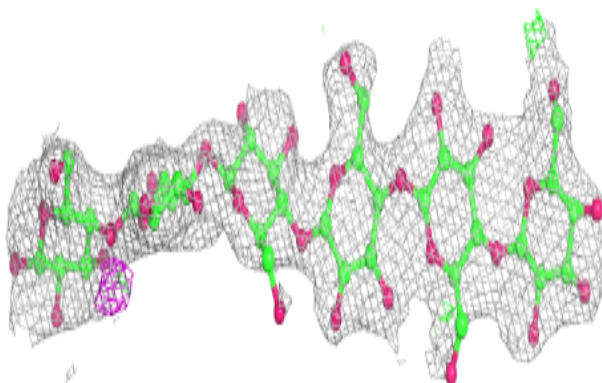


**Electron density around Chain O:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

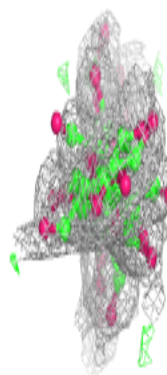
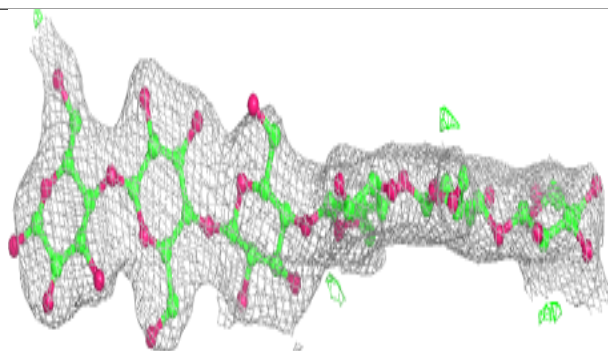
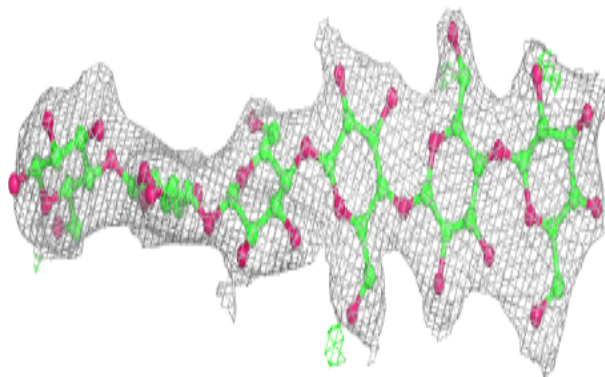
**Electron density around Chain P:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

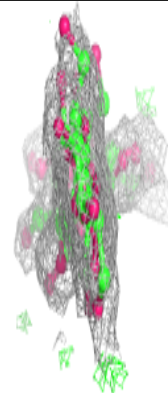
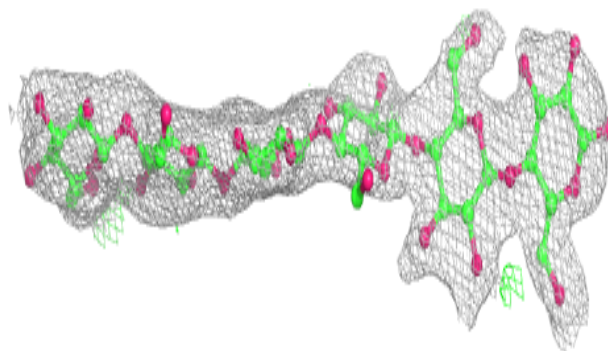
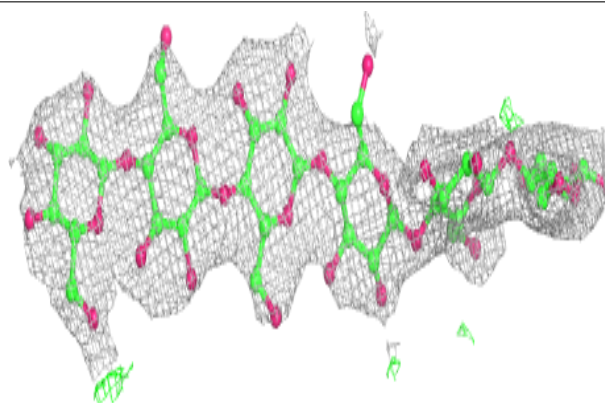


**Electron density around Chain Q:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

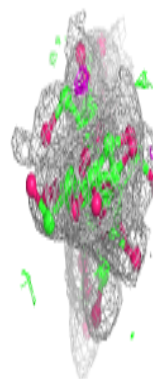
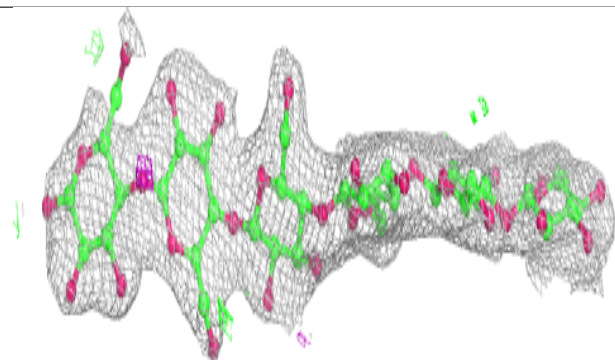
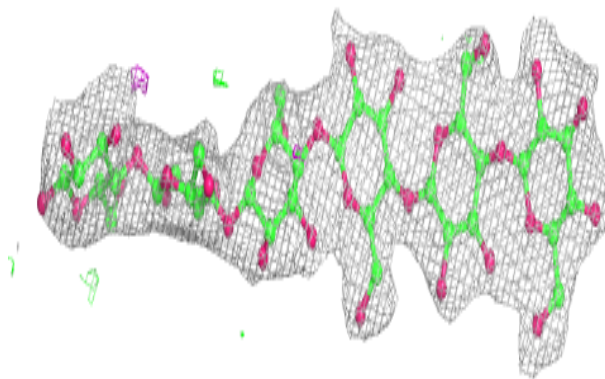
**Electron density around Chain R:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

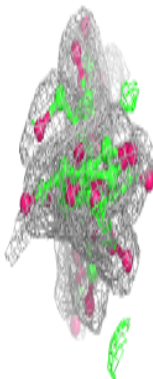
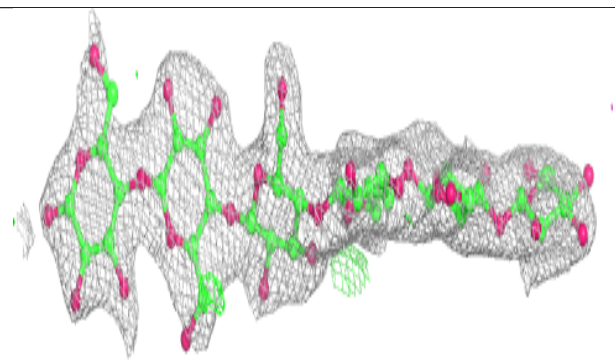
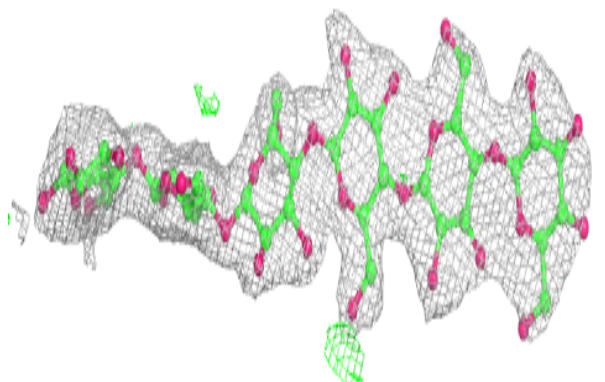


**Electron density around Chain S:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain T:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	EDO	G	610	4/4	0.73	0.17	54,57,57,58	0
5	ACT	H	608	4/4	0.78	0.16	66,69,70,74	0
7	EDO	E	609	4/4	0.79	0.19	52,55,56,56	0
7	EDO	G	611	4/4	0.79	0.16	54,55,56,57	0
6	PEG	B	609	7/7	0.82	0.21	49,53,61,62	0
7	EDO	D	609	4/4	0.84	0.17	56,63,63,65	0
6	PEG	A	609	7/7	0.85	0.15	52,57,64,66	0
5	ACT	I	608	4/4	0.86	0.20	52,53,56,57	0
6	PEG	B	610	7/7	0.86	0.12	56,57,60,61	0
5	ACT	E	608	4/4	0.86	0.23	42,51,53,64	0
7	EDO	C	609	4/4	0.87	0.18	51,53,53,53	0
7	EDO	H	609	4/4	0.87	0.16	52,54,55,57	0
5	ACT	D	608	4/4	0.88	0.21	53,53,54,57	0
7	EDO	E	612	4/4	0.88	0.15	65,67,68,68	0
7	EDO	G	612	4/4	0.88	0.21	44,46,50,51	0
7	EDO	G	608	4/4	0.88	0.23	41,47,50,52	0
5	ACT	J	608	4/4	0.89	0.14	48,49,54,58	0
5	ACT	B	608	4/4	0.89	0.17	38,42,43,50	0
5	ACT	F	608	4/4	0.89	0.14	51,55,57,57	0
7	EDO	G	609	4/4	0.89	0.11	50,57,58,59	0
7	EDO	C	610	4/4	0.91	0.16	47,50,51,51	0
7	EDO	E	610	4/4	0.91	0.20	43,47,50,52	0
6	PEG	J	609	7/7	0.91	0.12	52,52,56,56	0
6	PEG	A	608	7/7	0.92	0.30	36,45,58,62	0
7	EDO	I	609	4/4	0.92	0.12	54,57,58,59	0
7	EDO	B	612	4/4	0.93	0.11	54,54,55,55	0
5	ACT	A	607	4/4	0.93	0.17	54,56,58,60	0
5	ACT	C	608	4/4	0.94	0.16	47,51,54,55	0
7	EDO	E	611	4/4	0.94	0.12	48,49,52,53	0
4	MG	F	607	1/1	0.95	0.06	52,52,52,52	0
4	MG	C	607	1/1	0.95	0.10	50,50,50,50	0
4	MG	I	607	1/1	0.96	0.05	55,55,55,55	0
4	MG	D	607	1/1	0.96	0.09	44,44,44,44	0
4	MG	G	607	1/1	0.96	0.06	53,53,53,53	0
7	EDO	A	610	4/4	0.97	0.14	46,47,51,52	0
4	MG	A	606	1/1	0.97	0.12	45,45,45,45	0
7	EDO	C	611	4/4	0.97	0.15	36,37,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	E	607	1/1	0.98	0.12	54,54,54,54	0
4	MG	H	607	1/1	0.98	0.08	51,51,51,51	0
4	MG	B	607	1/1	0.99	0.09	48,48,48,48	0
7	EDO	B	611	4/4	0.99	0.12	36,37,37,39	0
4	MG	J	607	1/1	0.99	0.08	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.